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A Mathematical Introduction to the Wigner Formulation of Quantum Mechanics.

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Sunto. – *Il presente articolo è una rassegna di alcuni aspetti matematici fondamentali della formulazione Wigneriana della meccanica quantistica. A partire dagli assiomi della meccanica quantistica e della meccanica statistica quantistica viene motivata l'introduzione della trasformazione di Wigner e viene infine dedotta l'equazione di Wigner.*

Summary. – *The paper is devoted to review, from a mathematical point of view, some fundamental aspects of the Wigner formulation of quantum mechanics. Starting from the axioms of quantum mechanics and of quantum statistics, we justify the introduction of the Wigner transform and eventually deduce the Wigner equation.*

1. – Introduction.

The present notes are intended to give a brief introduction to the mathematical aspects of the Wigner formulation of quantum mechanics. We shall restrict our discussion to quantum mechanical systems with d degrees of freedom. By this we mean that we do not treat here spin-like degrees of freedom, identical particles systems, relativistic quantum mechanics, or quantum fields. To be more precise, we shall focus our attention on quantum systems whose states are described by the Hilbert space $L^2(\mathbb{R}^d, \mathbb{C})$. However, more general versions of the Wigner equation have been introduced for spin systems [2, 8, 10] and for second-quantized systems, [7, 15]. During the last decade, the mathematical community has devoted to Wigner equation and related topics an increasing interest. Two aspects of such interest, among many others, are worth to be underlined here: the use of Wign-

er equations to deduce and prove semiclassical limits [5, 16, 20, 21] and, from a more applied point of view, the use of Wigner equation for semiconductor devices modeling [11, 14, 22, 28]. It is also worth to remark that the Wigner equation itself brings interesting mathematical problems. For example, the well-posedness of the stationary Wigner equation with inflow-like boundary conditions has not been fully proved so far, even in the one-dimensional case, [1, 3, 4].

Since in the present paper we wish to focus our attention on founding and mathematical aspects, the point of view that we are going to adopt is that of an axiomatic exposition, which is not concerned with the *why* of things. We recommend the book of Mackey [19] to the reader interested to a careful discussion of the axioms of quantum mechanics.

The paper is organized as follows. In Section 2 we recall and briefly comment the fundamental axioms of quantum mechanics, concerning the description of physical states, observables, measurements and dynamics. In Section 3 we recall the concept of «quantization» of a classical system and illustrate the Weyl quantization rule. This topic is closely related to the Wigner formulation of quantum mechanics, as it will become apparent later on. Section 4 is devoted to motivate and introduce the axioms of statistical quantum mechanics, which are an extension of the axioms presented in Section 2. This is the main step to the defintion of Wigner transform, which is most naturally defined for mixed states, rather than pure states. In Section 5 we introduce the Wigner transform $\mathcal{W}$ as a unitary mapping of $L^2(\mathbb{R}^{2d}, \mathbb{C})$ into itself. We also define the «Wigner functions» as the image under $\mathcal{W}$ of the functions that belong to the physically meaningful subset of $L^2(\mathbb{R}^{2d}, \mathbb{C})$ representing mixed states. The axioms of statistical quantum mechanics are then revisited in such Wigner representation that shows interesting analogies with classical statistical mechanics. Finally, in Section 6 we discuss the «wignerization» of operators. The explicit expressions of two important categories of operators, namely the constant coefficient differential operators and the multiplication operators, will be computed. This allows us, starting from the quantum Liouville equation, to deduce the so-called Wigner equation, i.e., the dynamical equation for the Wigner functions.

2. – The axioms of quantum mechanics.

Let us consider a mechanical system with d degrees of freedom. The description that quantum mechanics (QM) gives of such system can be summarized under the form of four axioms.

AXIOM 2.1 (States of the system). – *The possible states of the system are represented by unitary vectors belonging to the Hilbert space*

$$(2.1) \qquad\qquad\qquad \mathcal{H} := L^2(\mathbb{R}^d, \mathbb{C}).$$

Such vectors are usually called «wave functions» of the system.

AXIOM 2.2 (Observable quantities). – *The physical observable quantities of the system (or, simply, «observables»), such as position coordinates, momentum coordinates, kinetic energy and so on, are represented by linear, self-adjoint operators on $\mathcal{H}$* [1].

AXIOM 2.3 (Measurements). – *The result of the measurement of an observable associated to the self-adjoint operator A, performed when the system is in the state $\psi \in \mathcal{H}$, is a random variable $X_{A,\psi}$. The law of $X_{A,\psi}$ is given by the spectral measure associated to A and ψ:*

$$(2.2) \qquad\qquad \mathrm{Prob}\,[X_{A,\psi} \in \mathcal{B}] = \langle \psi, \mathfrak{I}_{\mathcal{B}}(A)\,\psi \rangle$$

for all Borel subsets $\mathcal{B}$ of $\mathbb{R}$.

In the above equation, $\langle \cdot, \cdot \rangle$ denotes the standard Hermitian product of $\mathcal{H}$

$$(2.3) \qquad\qquad \langle \psi, \phi \rangle := \int_{\mathbb{R}^d} \overline{\psi}(x)\,\phi(x)\,dx$$

and $\mathfrak{I}_{\mathcal{B}}$ denotes the indicator function of the Borel set $\mathcal{B}$:

$$(2.4) \qquad\qquad \mathfrak{I}_{\mathcal{B}}(x) := \begin{cases} 1, & \text{if } x \in \mathcal{B} \\ 0, & \text{if } x \notin \mathcal{B} \end{cases}$$

We recall that the spectral theorem [24] defines a self-adjoint operator $f(A)$ for any Borel-measurable function $f : \mathbb{R} \to \mathbb{R}$ and any self-adjoint operator A. In particular, if f is bounded, then $f(A)$ is a bounded operator and if $f \geq 0$, then $f(A)$ is a positive operator. It turns out that, if ψ belongs to the domain $\mathcal{D}(A)$ of A, then the random variable $X_{A,\psi}$ has finite expectation and

$$(2.5) \qquad\qquad \mathrm{Expect}\,[X_{A,\psi}] = \langle \psi, A\psi \rangle.$$

The last axiom we are going to consider concerns the time evolution of the system.

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[1] We remark that an observable A is not necessarily a bounded operator and, therefore, a domain $\mathcal{D}(A) \subset \mathcal{H}$ should always be specified.

AXIOM 2.4 (Evolution). – *Let H denote the self-adjoint operator, called «Hamiltonian», associated to the observable «total energy». If at time t_0 the system is in the state ψ_0, then, at any other time $t \in \mathbb{R}$ the system is in the state*

$$(2.6) \qquad \psi(t) = e^{-\frac{i}{\hbar}(t - t_0) H} \psi_0.$$

In eq. (2.6), *the one-parameter family* $e^{-\frac{i}{\hbar} t H}$, $t \in \mathbb{R}$, *is the unitary group of transformations generated by* H, [24]. *The symbol $\hbar$ denotes Planck's constant divided by* 2π. *The differential version of eq. (2.6) has the form of an evolution equation in the space* $\mathcal{H}$, *namely*

$$(2.7) \qquad i\hbar \frac{d}{dt} \psi(t) = H\psi(t), \quad t \in \mathbb{R},$$

which is the abstract form of Schrödinger equation.

Let us make some comments on Axioms 2.1-2.4. The first Axiom tells us how QM describes physical states ([2]). Contrarily to classical mechanics, where the state is a distribution in phase-space, having, therefore, a direct physical meaning, a quantum mechanical state ψ does not possess such direct physical meaning. However ψ encloses *all* the physical information, which has to be «extracted», so to speak, from ψ. Axioms 2.2 and 2.3 constitute the general rule to extract physical information from the wave function. In particular, they tell us that such information has an intrinsically *probabilistic* nature. The randomness of nature at the quantum scale is something *unavoidable*, which do not disappear even if we would use an ideal instrument of infinite precision. Thus, the knowledge of the distribution of the random variable $X_{A,\psi}$ is the best we can expect from the theory and from the experiments.

It is important to notice at this point that the already mentioned spectral theorem fournishes the following «consistency» rule:

$$(2.8) \qquad f(X_{A,\psi}) = X_{f(A),\psi}$$

which holds for any Borel-measurable function $f : \mathbb{R} \to \mathbb{R}$ and any self-adjoint operator A.

REMARK 2.1. – So far, nothing has been said about the *simultaneous* measurement of two or more observables. Indeed, Axiom 2.3 should be completed by the following statement: *a set of «commuting observables» (i.e., a set of k observables whose associated self-adjoint operators $A_1, \dots A_k$ commmute*

([2]) We remark that here we should have been speaking of *pure* states; in Sec. 4 we shall see that a more general class of states, the *mixed states* which are needed in quantum statistics, can be introduced.

pairwise) can be measured simultaneously in any state ψ and the result of the measurement is a multiple random variable $(X_{A_1, \psi}, \ldots, X_{A_k, \psi})$ whose law is given by ([3])

$$(2.9) \qquad \text{Prob}\,[(X_{A_1, \psi}, \ldots, X_{A_k, \psi}) \in \mathcal{B}_1 \times \ldots \times \mathcal{B}_k] = \langle \psi, \mathfrak{I}_{\mathcal{B}_1}(A_1) \ldots \mathfrak{I}_{\mathcal{B}_k}(A_k)\psi \rangle,$$

where $\mathcal{B}_1, \ldots, \mathcal{B}_k$ are Borel sets in $\mathbb{R}$. In the case of non-commuting observables, the possibility of simultaneous measurement may be state-dependent or even undefined at all (for a careful discussion of this point see Ref. [23]). ■

Finally, Axiom 2.4 tells us that the evolution of the system is *deterministic*: once the quantum mechanical state is known at a certain time, all the past and future states of the system are determined. Since the operators $\mathrm{e}^{-\frac{i}{\hbar}tH}$ are unitary, the norm of ψ_0 is preserved during the evolution.

3. – Quantization.

The presentation of QM developed so far is rather formal and, indeed, Axioms 2.1-2.4 describe quite general aspects of the theory, which are common to other quantum theories. In order to make the axioms really «work», the crucial point is to specify the correspondence

$$\text{observable quantities} \rightarrow \text{self-adjoint operators}\,.$$

Such specification is the so-called *quantization*. To be more precise, let us recall that a physical observable is described in classical mechanics (CM) by a real function $\gamma = \gamma(r, p)$, defined on the phase space $\mathbb{R}^{2d} = \mathbb{R}^d_r \times \mathbb{R}^d_p$. For example, the kinetic energy of a free particle of mass m is given by the function $\gamma(r, p) = p^2/2m$ (and $d = 3$, in this case). From the point of view of quantization, such function γ is usually termed the *classical symbol* (or simply the «symbol») of the observable under consideration.

DEFINITION 3.1. – *We call «quantization» a procedure that allows to associate to a classical symbol γ a self-adjoint operator A_γ, that describes in QM the same physical quantity represented in CM by γ.*

The quantization procedure starts from a *fundamental quantization*, i.e., the quantization of the symbols $\gamma(r, p) = r$, associated to the observable «position», and $\gamma(r, p) = p$, associated to the observable «momentum».

([3]) We recall that the probabilities of the «rectangular» Borel sets, of the form $\times_{j=1}^{k}\mathcal{B}_j$, uniquely defines the probabilities of all the Borel sets in $\mathbb{R}^k$. Thus, the law of the multiple random variable $(X_{A_1, \psi}, \ldots, X_{A_k, \psi})$ is completely determined by (2.9) (see, e.g., Ref. [6]).
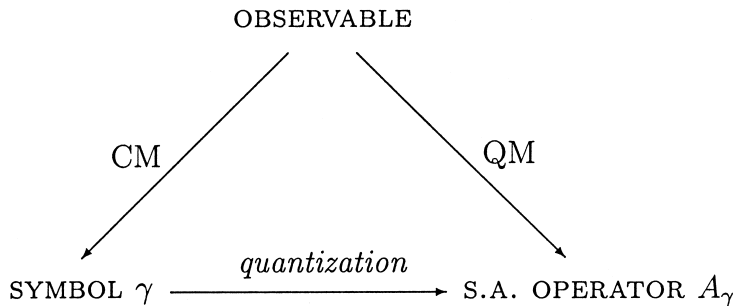
Figure 1. – The quantization scheme.

The fundamental quantization rests on physical experience and prescribes that to the symbols r and p correspond the self-adjoint operators A_r and A_p defined as follows:

$$(3.1) \qquad (A_r \psi)(x) := x\psi(x), \quad x \in \mathbb{R}^d$$

for all $\psi \in \mathcal{D}(A_r) := \{\psi \in \mathcal{H} \,|\, A_r \psi \in \mathcal{H}\}$, and

$$(3.2) \qquad (A_p \psi)(x) := -i\hbar \frac{\partial}{\partial x} \psi(x), \quad x \in \mathbb{R}^d$$

for all $\psi \in \mathcal{D}(A_p) := \{\psi \in \mathcal{H} \,|\, A_p \psi \in \mathcal{H}\}$. Note that r and p are vectors of symbols and, correspondingly, eqs. (3.1) and (3.2) define vectors of operators. For $j = 1, 2, \dots, d$, each component r_j of r and p_j of p is a scalar observable and, correspondingly, each component A_{r_j} of A_r and A_{p_j} of A_p is a self-adjoint operator. Note also that we used the notation

$$\frac{\partial}{\partial x} := \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \dots, \frac{\partial}{\partial x_d} \right).$$

An interesting fact is that the operators A_r and A_p transform into each other, by similarity, through the Fourier transform

$$(3.3) \qquad (\mathcal{F}\psi)(p) := (2\pi\hbar)^{-d/2} \int_{\mathbb{R}^d} \psi(x) \, e^{-ix \cdot p/\hbar} \, dx \ .$$

Since the components of A_r are pairwise commuting operators, according to Axiom 2.3 and Remark 2.1 the result of a measurement of the position, when our system is in the state ψ, is a multiple random variable $X_{A_r, \psi} = (X_{A_{r_1}, \psi}, \dots, X_{A_{r_d}, \psi})$ whose law is given by (2.9). Each component A_{r_j} of A_r is such that $[A_{r_j} \psi](x) = x_j \psi(x)$ and thus, if $\mathcal{B}_j$ is any Borel subset of $\mathbb{R}$, from the

spectral theorem we have that the bounded operator $\Im_{\mathcal{B}_j}(A_{r_j})$ is given by

$$(3.4) \qquad [\Im_{\mathcal{B}_j}(A_{r_j})\,\psi](x) = \Im_{\mathcal{B}_j}(x_j)\,\psi(x), \qquad x \in \mathbb{R}^d,$$

for every $\psi \in \mathcal{H}$. Therefore, for any rectangular Borel set $\mathcal{B} \subset \mathbb{R}^d$ of the form $\mathcal{B} = \times_{j=1}^d \mathcal{B}_j$, from (2.9) and (3.4) we obtain

$$\mathrm{Prob}\,[X_{A_r,\,\psi} \in \mathcal{B}] = \langle \psi,\, \Im_{\mathcal{B}_1}(A_{r_1})\,\Im_{\mathcal{B}_2}(A_{r_2})\,\dots\,\Im_{\mathcal{B}_d}(A_{r_d})\,\psi \rangle =$$

$$\int_{\mathbb{R}^d} \prod_{j=1}^d \Im_{\mathcal{B}_j}(x_j)\,\overline{\psi(x)}\,\psi(x)\,dx = \int_{\mathbb{R}^d} \Im_{\mathcal{B}}(x)\,\overline{\psi(x)}\,\psi(x)\,dx = \int_{\mathcal{B}} |\psi(x)|^2\,dx\,.$$

Hence, we can conclude that the (multiple) random variable $X_{A_r,\,\psi}$ is absolutely continuous and $|\psi(x)|^2$ is its density. We therefore have the well known fact that *the squared modulus of the wave function is the density of the random variable «measurement of position»*.

Analogously, let us consider the momentum operator A_p, whose components $A_{p_j} = -i\hbar\dfrac{\partial}{\partial x_j}$, $j = 1, 2, \dots, d$, commute pairwise. According to Axiom 2.3 and Remark 2.1 the result of a measurement of the momentum, when our system is in the state ψ, is a multiple random variable $X_{A_p,\,\psi} = (X_{A_{p_1},\,\psi}, \dots, X_{A_{p_d},\,\psi})$. In order to apply (2.9) to obtain the law of $X_{A_p,\,\psi}$, we observe that the spectral theorem implies that, for any given Borel set $\mathcal{B}_j \in \mathbb{R}$, the Fourier-transformed operator $\mathcal{F}\Im_{\mathcal{B}_j}(A_{p_j})\,\mathcal{F}^{-1}$ acts as the multiplication by $\Im_{\mathcal{B}_j}(p_j)$, i.e.,

$$(3.5) \qquad [\mathcal{F}\Im_{\mathcal{B}_j}(A_{p_j})\,\mathcal{F}^{-1}\psi](p) = \Im_{\mathcal{B}_j}(p_j)\,\psi(p), \qquad p \in \mathbb{R}^d,$$

for every $\psi \in \mathcal{H}$. Thus, according to (2.9) and (3.5), for any rectangular Borel set $\mathcal{B} = \times_{j=1}^d \mathcal{B}_j \subset \mathbb{R}^d$ and for every $\psi \in \mathcal{H}$ we can write

$$\mathrm{Prob}\,[X_{A_p,\,\psi} \in \mathcal{B}] = \langle \psi,\, \Im_{\mathcal{B}_1}(A_{p_1})\Im_{\mathcal{B}_2}(A_{p_2})\,\dots\,\Im_{\mathcal{B}_d}(A_{p_d})\,\psi \rangle =$$

$$\langle \mathcal{F}\psi,\, \mathcal{F}\Im_{\mathcal{B}_1}(A_{p_1})\,\mathcal{F}^{-1}\mathcal{F}\Im_{\mathcal{B}_2}(A_{p_2})\,\mathcal{F}^{-1}\dots\,\mathcal{F}\Im_{\mathcal{B}_d}(A_{p_d})\,\mathcal{F}^{-1}\mathcal{F}\psi \rangle =$$

$$\int_{\mathbb{R}^d} \prod_{j=1}^d \Im_{\mathcal{B}_j}(p_j)\,|(\mathcal{F}\psi)(p)|^2\,dp = \int_{\mathcal{B}} |(\mathcal{F}\psi)(p)|^2\,dp.$$

Hence, the (multiple) random variable $X_{A_p,\,\psi}$ is absolutely continuous and $|(\mathcal{F}\psi)(p)|^2$ is its density. Therefore, *the squared modulus of the Fourier transform of the wave function is the density of the random variable «measurement of momentum»*.

Starting from the fundamental quantization, we need a recipe to quantize all the other observables. If the symbol γ is a function of the sole r, or of the sole p, the consistency relation (2.8) implies that the only possible quantization

rule is given by the spectral theorem:

$$(3.6) \qquad\qquad A_{f(r)} = f(A_r), \qquad A_{g(p)} = g(A_p),$$

for every measurable $f = f(r)$ and $g = g(p)$. But for a general $\gamma = \gamma(r, p)$ we immediately step into a difficulty. In fact, the lack of commutativity between A_r and A_p makes unclear any «naive» attempt to establish a correspondence $\gamma \to A_\gamma$. Consider, for example, the symbol $\gamma(r, p) = r^2 p$: how do we quantize it? It is evident that there are many possible choices, such as $A_r^2 A_p$, $A_r A_p A_r$, $A_p A_r^2$ or also $(A_r^2 A_p + A_r A_p A_r + A_p A_r^2)/3$, and so on. It is immediate to see that, indeed, not all these expressions define the same operator.

We have, therefore, to choose a unambiguous quantization rule. The requirements for such quantization are the following:

(Q1)   it must associate to any symbol γ (with the opportune regularity) a unique self-adjoint operator A_γ;

(Q2)   it must respect the fundamental quantization, defined by (3.1), (3.2) and (3.6);

(Q3)   it must reduce quantum mechanics to classical mechanics in the «classical limit» $\hbar \to 0$.

A commonly accepted rule which satisfies the requirements (Q1)-(Q3) is the *Weyl quantization*, [26], defined by

$$(3.7) \qquad (A_\gamma \psi)(x) := (2\pi\hbar)^{-d} \int_{\mathbb{R}_y^d \times \mathbb{R}_p^d} \gamma\left(\frac{x+y}{2}, p\right) \psi(y)\, e^{\frac{i}{\hbar}(x-y)\cdot p}\, dy\, dp$$

for all $x \in \mathbb{R}^d$. We remark that the above expression is only formal since we did not specify the required properties of the symbol, neither the domain of A_γ. For a rigorous description of Weyl quantization we refer the reader to [13, 26]. The above defined operator A_γ is sometimes indicated with the suggestive notation $\gamma(A_r, A_p)$. As an exercise, the reader may check that, at least formally, the quantization properties (Q1) and (Q2) are satisfied and compute the Weyl quantization of the symbol $r^2 p$, with $d = 1$ ([4]).

REMARK 3.1. – We have seen that, thanks to Weyl quantization, every classical observable has its counterpart in QM. However, the converse is not true: there exist quantum observables (i.e., self-adjoint operators) that are not the quantization of any classical quantity.   ∎

As an important illustration of the above Remark 3.1, let us consider for every wave function ψ the orthogonal projection P_ψ onto the subspace of $\mathcal{H}$

([4]) Solution: $A_{r^2 p} = A_r A_p A_r = (A_x^2 A_p + A_p A_x^2)/2$.

spanned by ψ:

$$(3.8) \qquad P_\psi := \langle \psi, \cdot \rangle \, \psi \, .$$

It is easy to see that P_ψ is self-adjoint and that its spectrum is composed by the two eigenvalues 1 and 0 corresponding to the eigenspaces $P_\psi \mathcal{H}$ and $(I - P_\psi) \, \mathcal{H}$, respectively. Thus, according to Axioms 2.2 and 2.3, to P_ψ there corresponds an «observable quantity» that takes the value 1 with certainty if and only if the system is in state ψ. We shall, therefore, interpret P_ψ as the observable quantity «beeing in state ψ», which has the possible values 1 (=yes) and 0 (=no). The observable P_ψ has no classical counterpart. We also note that, since there is a 1-1 correspondence between states an projections, we should also identify the two objects. Such point of view will be prevalent in quantum statistics (ses Sec. 4).

We end this section by noting that, for every self-adjoint operator A and for every $\psi \in \mathcal{D}(A)$ the following equality holds

$$(3.9) \qquad \langle \psi, A\psi \rangle = \mathrm{Tr} \, (P_\psi A),$$

where Tr denotes the operator trace ([5]). From eq. (2.2), therefore, we have that all the physically relevant informations of the theory (probabilities and expectations) can be expressed as traces of operators of the form (3.9).

4. – Statistical quantum mechanics.

The wave function of a quantum mechanical systems represents the «best possible» physical knowledge we can have on the system and, as we have seen in Sec. 2, such «best possible» knowledge is «uncertain» in its intrinsic nature. However in many occasions we cannot expect to have such complete, although probabilistic, information. This is the typical situation, for example, when the number of degrees of freedom is very high, as in many-particles systems. In such cases we are forced to describe our system by something which is different from the wave function that we have considered so far and we say that we are doing *statistical quantum mechanics*, or *quantum statistics*, [12, 23].

In order to see which kind of object has to substitute the wave function in statistical QM, let us consider the case of a system $\mathcal{S}$ with d degrees of freedom which is a subsystem of a larger system $\mathcal{S}'$ with $d + D$ degrees of freedom (where d is usually small and D very large as in the case of a single particle

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([5]) We recall the definition of trace. If $\mathcal{H}$ is a separable Hilbert space with Hermitian product $\langle \cdot, \cdot \rangle$ and $\{\phi_k\}_{k=1}^{\infty}$ is an orthonormal basis of $\mathcal{H}$, the trace of a positive operator A is $\mathrm{Tr}\,(A) := \sum_{k=1}^{\infty} \langle \phi_k, A\phi_k \rangle$. Such definition does not depend on the choice of the basis and it is extended to all operators such that $\mathrm{Tr}\,(|A|) < +\infty$ (see Ref. [24]).

dispersed into a gas of many other similar particles). Let $\Psi = \Psi(x, \eta)$ be the wave function of the large system $\mathcal{S}'$, with $x \in \mathbb{R}_x^d$ and $\eta \in \mathbb{R}_\eta^D$. From Fubini's theorem we have that, for almost every $\eta \in \mathbb{R}_\eta^D$, the function $x \mapsto \psi_\eta(x) := \Psi(x, \eta)$ is a wave function for the small subsystem $\mathcal{S}$. Now, consider an observable A which involves only the first d coordinates x of Ψ. Note that A can be regarded as acting on $L^2(\mathbb{R}_x^d \times \mathbb{R}_\eta^D, \mathbb{C})$ as well as on $L^2(\mathbb{R}_x^d, \mathbb{C})$. Such operator A represents a physical quantity possessed by the subsystem $\mathcal{S}$.

If we formally compute the expected value of A in the state Ψ by using (3.9) we obtain

$$(4.1) \qquad \langle \Psi, A\Psi \rangle = \int_{\mathbb{R}_\eta^D} \langle \psi_\eta, A\psi_\eta \rangle \, d\eta = \int_{\mathbb{R}_\eta^D} \mathrm{Tr}\,(P_{\psi_\eta} A) \, d\eta = \mathrm{Tr}\left(\int_{\mathbb{R}_\eta^D} P_{\psi_\eta} \, d\eta \, A \right),$$

where in the first and in the second term $\langle \cdot, \cdot \rangle$ indicates the Hermitian products in $L^2(\mathbb{R}_x^d \times \mathbb{R}_\eta^D, \mathbb{C})$ and in $\mathcal{H} = L^2(\mathbb{R}_x^d, \mathbb{C})$, respectively. The above equation shows that the expected value of A can be expressed as the trace of ϱA, where the operator $\varrho = \int_{R_\eta^D} P_{\psi_\eta} \, d\eta$ is defined by

$$(4.2) \qquad \varrho\psi := \int_{\mathbb{R}_\eta^D} P_{\psi_\eta} \psi \, d\eta, \quad \psi \in \mathcal{H}.$$

Before going on, it is worth to make a brief digression in order to recall some basic facts about Hilbert-Schmidt and density operators. We firstly recall that a bounded operator ϱ on $\mathcal{H}$ is a Hilbert-Schmidt (HS) operator if

$$(4.3) \qquad \|\varrho\|_{\mathrm{HS}} = (\langle \varrho, \varrho \rangle_{\mathrm{HS}})^{1/2} := (\mathrm{Tr}\,(\varrho\varrho^*))^{1/2}$$

is finite. The space of HS-operators on $\mathcal{H}$, denoted by $\mathfrak{J}_2(\mathcal{H})$, is a Hilbert space with respect to the above norm and Hermitian product.

The proofs of Theorems 4.1 and 4.2 below can be found in Ref. [24].

THEOREM 4.1. – *An operator ϱ on $\mathcal{H}$ is HS if and only if a function $\varrho(x, y)$, belonging to $L^2(\mathbb{R}_x^d \times \mathbb{R}_y^d, \mathbb{C})$ exists such that*

$$(4.4) \qquad (\varrho\psi)(x) = \int_{\mathbb{R}_y^d} \varrho(x, y) \, \psi(y) \, dy$$

for all $\psi \in \mathcal{H}$. Moreover, the correspondence between the operator ϱ and the integral kernel $\varrho(x, y)$ is an isomorphism between the Hilbert spaces $\mathfrak{J}_2(\mathcal{H})$ and $L^2(\mathbb{R}_x^d \times \mathbb{R}_y^d, \mathbb{C})$.

The Hilbert spaces $\mathfrak{J}_2(\mathcal{H})$ and $L^2(\mathbb{R}_x^d \times \mathbb{R}_y^d, \mathbb{C})$ are both isomorphic to $\mathcal{H} \otimes \mathcal{H}$. In the following, for the sake of simplicity, we shall make a systematic

identification of the three spaces. In particular, the same symbol ϱ will be used to indicate both the HS-operator and its kernel. Moreover, we shall allow a double interpretation of the tensor product $\psi \otimes \phi$ of ψ, $\phi \in \mathcal{H}$:

1. as a HS-operator:

$$(4.5) \qquad \psi \otimes \phi := \langle \phi, \cdot \rangle \, \psi$$

2. as a function (kernel of the above operator):

$$(4.6) \qquad (\psi \otimes \phi)(x, y) := \psi(x) \, \overline{\phi(y)}, \quad x, y \in \mathbb{R}^d.$$

We now focus our attention on density operators, which are a special class of HS-operators.

DEFINITION 4.1. – *A HS-operator ϱ on $\mathcal{H}$ is called* density operator *if it has the following properties:*

  (i) *ϱ is self-adjoint;*

  (ii) *ϱ is positive* (^{6});

  (iii) $\mathrm{Tr}\,(\varrho) = 1$.

The following characterization is a fundamental point in the analysis of density operators.

THEOREM 4.2. – *An operator ϱ on $\mathcal{H}$ is a density operator if and only if there exist a complete orthonormal system $\{\phi_j\}_{j=1}^{\infty}$ of $\mathcal{H}$ and a sequence of non-negative real numbers $\{\alpha_j\}_{j=1}^{\infty}$, with $\sum\limits_{j=1}^{\infty} \alpha_j = 1$, such that*

$$(4.7) \qquad \varrho = \sum_{j=1}^{\infty} \alpha_j \, \phi_j \otimes \phi_j.$$

Moreover, every ϕ_j is an eigenfunction of ϱ with eigenvector α_j and $\|\varrho\|_{\mathrm{HS}}^2 = \sum\limits_{j=1}^{\infty} \alpha_j^2$.

It is now time to come back to the operator $\varrho = \int\limits_{\mathbb{R}_\eta^D} P_{\psi_\eta} \, d\eta$ which we have met at the beginning of this section. We recall that $\Psi \in L^2(\mathbb{R}_x^d \times \mathbb{R}_\eta^D, \mathbb{C})$ is a wave function of the «large» system $\mathcal{S}'$ and $\psi_\eta := \Psi(\cdot, \eta)$ is a wave function of the «small» subsystem $\mathcal{S}$.

PROPOSITION 4.1. – *The operator ϱ defined by (4.2) is a density operator on $\mathcal{H}$.*

(^{6}) We recall that ϱ is «positive» if $\langle \psi, \varrho\psi \rangle \geq 0$ for all $\psi \in \mathcal{H}$.

PROOF. – We have to prove that ϱ is HS and that (i), (ii), (iii) of Definition 4.1 hold.

(i) From (4.2) and (3.8) we have, for any given $\psi \in \mathcal{H}$,

$$(\varrho\psi)(x) = \int\limits_{\mathbb{R}_\eta^D} \int\limits_{\mathbb{R}_y^d} \overline{\psi_\eta(y)}\, \psi_\eta(x)\, \psi(y)\, dy\, d\eta = \int\limits_{\mathbb{R}_y^d} \varrho(x, y)\, \psi(y)\, dy,$$

where

$$\varrho(x, y) := \int\limits_{\mathbb{R}_\eta^D} \overline{\psi_\eta(y)}\, \psi_\eta(x)\, d\eta = \int\limits_{\mathbb{R}_\eta^D} \overline{\Psi(y, \eta)}\, \Psi(x, \eta)\, d\eta\ .$$

By using Hölder's inequality we obtain

$$\int\limits_{\mathbb{R}_x^d \times \mathbb{R}_y^d} |\varrho(x, y)|^2\, dx\, dy \leq \int\limits_{\mathbb{R}_x^d \times \mathbb{R}_\eta^D} |\Psi(x, \eta)|^2\, dx\, d\eta \int\limits_{\mathbb{R}_y^d \times \mathbb{R}_\eta^D} |\Psi(y, \eta)|^2\, dy\, d\eta \leq 1,$$

since Ψ is a wave function and, as such, it is normalized to unity. Thus, ϱ is a Hilbert-Schmidt operator (see Theorem 4.1) and the self-adjointness follows immediately from $\overline{\varrho(x, y)} = \varrho(y, x)$.

(ii) For any given $\psi \in \mathcal{H}$ note that

$$\langle \psi, \varrho\psi \rangle = \int\limits_{\mathbb{R}_\eta^D} \left| \int\limits_{\mathbb{R}_x^d} \Psi(x, \eta)\, \overline{\psi(x)}\, dx \right|^2 d\eta \geq 0\ ,$$

which means, by definition, that ϱ is positive. (see, e.g., Ref. [24]).

(iii) Let $\{e_i\}_{i=1}^\infty$ be a complete orthonormal system of $\mathcal{H}$. For almost every $\eta \in \mathbb{R}_\eta^D$ we have

$$\sum_{i=1}^\infty |\langle e_i, \psi_\eta \rangle|^2 = \int\limits_{\mathbb{R}_x^d} |\psi_\eta(x)|^2\, dx = \int\limits_{\mathbb{R}_x^d} |\Psi(x, \eta)|^2\, dx$$

and, therefore,

$$\mathrm{Tr}\,(\varrho) = \sum_{i=1}^\infty \langle e_i, \varrho e_i \rangle = \sum_{i=1}^\infty \int\limits_{\mathbb{R}_\eta^D} \left| \int\limits_{\mathbb{R}_x^d} \Psi(x, \eta)\, \overline{e_i(x)}\, dx \right|^2 d\eta =$$

$$= \sum_{i=1}^\infty \int\limits_{\mathbb{R}_\eta^D} |\langle e_i, \psi_\eta \rangle|^2\, d\eta = \int\limits_{\mathbb{R}_x^d \times \mathbb{R}_\eta^D} |\Psi(x, \eta)|^2\, dx\, d\eta = 1,$$

where we used again the fact that Ψ is a wave function. ∎

We remark that putting $\psi(x) := \int\limits_{\mathbb{R}_\eta^D} \Psi(x, \eta)\, d\eta$ does *not* define a wave function for the subsystem $\mathcal{S}$ since, in general, such ψ does not belong

to $\mathcal{H}$. *The integration with respect to η of a wave function $\Psi(x, \eta)$ of the large system S' has a well defined meaning only as an operator.*

All this considered, we are led to generalize Axiom 2.1 by defining a more general class of quantum states.

AXIOM 4.1 (Mixed states of the system). – *The* mixed states *of a quantum mechanical systems, whose wave functions belong to $\mathcal{H}$, are represented by the density operators acting on $\mathcal{H}$. The mixed state ϱ is said to be a* pure state *if and only if a wave function $\psi \in \mathcal{H}$ exists such that $\varrho = P_\psi$ (see (3.8)).*

The integral kernel $\varrho(x, y)$ of a density operator ϱ (see Theorem 4.1) is usually called *density matrix*. Note that, according to (4.5) and (4.6), the pure state $\varrho = P_\psi$ has the form $\psi \otimes \psi$ and its density matrix of is $\varrho(x, y) = \psi(x)\, \overline{\phi(y)}$.

REMARK 4.1. – We can restate Theorem 4.2 by saying that *mixed states are convex combinations, possibly infinite, of pure states.*

We are led by (2.2), (3.9) and (4.1) to extend Axiom 2.3 as follows.

AXIOM 4.2 (Measurements in mixed states). – *The result of a measurement of the observable A, performed when the system is in the mixed state ϱ, is a random variable $X_{A, \varrho}$ with law given by*

$$(4.8) \qquad \mathrm{Prob}\,[X_{A, \varrho} \in \mathcal{B}] = \mathrm{Tr}\,(\varrho\, \mathfrak{I}_{\mathcal{B}}(A))$$

for all Borel subset $\mathcal{B}$ of $\mathbb{R}$.

We recall that $\mathfrak{I}_{\mathcal{B}}(A)$ is a bounded operator and, therefore, the trace appearing in (4.8) is finite (see Ref. [24], Theorem VI.19). The discussion of the cases in which $X_{A, \varrho}$ has finite expectation, given by

$$(4.9) \qquad \mathrm{Expect}\,[X_{A, \varrho}] = \mathrm{Tr}\,(\varrho A),$$

is more delicate and goes beyond the scope of the present notes.

We now turn our attention to dynamics; in fact, we still have to extend Axiom 2.4 to the evolution of mixed states. Recall that the evolution of a pure state is given by eq. (2.6). Therefore, if we use the operatorial form $\psi \otimes \psi$ to describe pure states, we obtain from (2.6) and (4.5)

$$\psi(t) \otimes \psi(t) = (\mathrm{e}^{-\frac{i}{\hbar}(t-t_0)H}\psi_0) \otimes (\mathrm{e}^{-\frac{i}{\hbar}(t-t_0)H}\psi_0) = \langle \mathrm{e}^{-\frac{i}{\hbar}(t-t_0)H}\psi_0, \cdot \rangle\, \mathrm{e}^{-\frac{i}{\hbar}(t-t_0)H}\psi_0 =$$

$$\langle \psi_0, \mathrm{e}^{\frac{i}{\hbar}(t-t_0)H}(\cdot) \rangle\, \mathrm{e}^{-\frac{i}{\hbar}(t-t_0)H}\psi_0 = \mathrm{e}^{-\frac{i}{\hbar}(t-t_0)H}(\psi_0 \otimes \psi_0)\, \mathrm{e}^{\frac{i}{\hbar}(t-t_0)H},$$

where the unitarity of $\mathrm{e}^{-\frac{i}{\hbar}tH}$ was used. Since every mixed state has the

form (4.7), by linearity we are led from the previous calculation to extend Axiom 2.4 in the following way.

AXIOM 4.3 (Evolution of mixed states). – *Let H be the Hamiltonian of the system. If at time t_0 the system is in the mixed state ϱ_0, then, at any other time $t \in \mathbb{R}$ the system is in the mixed state*

$$(4.10) \qquad \varrho(t) = e^{-\frac{i}{\hbar}(t-t_0)H} \varrho_0 \, e^{\frac{i}{\hbar}(t-t_0)H}.$$

By formally differentiating eq. (4.10) with respect to time we obtain the differential version of (4.10), called *quantum Liouville equation*:

$$(4.11) \qquad i\hbar \frac{d}{dt}\varrho(t) = [H, \varrho(t)], \quad t \in \mathbb{R},$$

where $[A, B] := AB - BA$ is the commutator between the operators A and B. The quantum Liouville equation (4.11) is the mixed-state version of Schrödinger equation (2.7).

5. – The Wigner transform.

The Wigner transform was introduced by E. Wigner in 1932, [27]. It is a «phase-space like» representation of (statistical) QM. By this we mean, exactly, that the Wigner transform is a unitary mapping that *takes a mixed state into something that is formally similar to a distribution in phase-space*. In QM, of course, it cannot exist a thing like a «distribution in phase space» since, owing to Heisenberg's uncertainity relation, the position of the system in phase-space is an undefined quantity. The analogy of the Wigner representation of QM with the classical statistical mechanics, however, turns out to be useful and very suggestive in many situations, [8, 22, 25]. Nevertheless, it is worth to remark that the Wigner transform constitutes also an useful tool in other branches of pure and applied mathematics, [9, 10, 13, 16].

In the last section we introduced the main objects of statistical QM, which are density operators on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}_x^d, \mathbb{C})$. We have also seen that such operators are in a 1-1 isometric correspondence with their integral kernels belonging to $L^2(\mathbb{R}_x^d \times \mathbb{R}_y^d, \mathbb{C}) \sim \mathcal{H} \otimes \mathcal{H}$ and, therefore, kernels and operators can be canonically identified.

Let us consider the map $\mathcal{R}$ of $L^2(\mathbb{R}_x^d \times \mathbb{R}_y^d, \mathbb{C})$ into $L^2(\mathbb{R}_r^d \times \mathbb{R}_\xi^d, \mathbb{C})$ given by

$$(5.1) \qquad (\mathcal{R}\varrho)(r, \xi) := \varrho\left(r + \frac{\hbar}{2}\xi, \, r - \frac{\hbar}{2}\xi\right),$$

corresponding to the change of variables $(x, y) \mapsto (r, \xi)$

$$
\begin{cases} r = \dfrac{x+y}{2} \\[2mm] \xi = \dfrac{x-y}{\hbar} \end{cases} \qquad \begin{cases} x = r + \dfrac{\hbar}{2}\xi \\[2mm] y = r - \dfrac{\hbar}{2}\xi \,. \end{cases}
$$

A simple computation yields

$$
(5.3) \qquad \langle \mathscr{R}\varrho_1, \mathscr{R}\varrho_2 \rangle = \hbar^{-d} \langle \varrho_1, \varrho_2 \rangle
$$

for all ϱ_1, ϱ_2, i.e., $\mathscr{R}$ is a unitary transformation from $L^2(\mathbb{R}^{2d}, \mathbb{C})$ into itself, apart from the constant factor $\hbar^{-d}$.

Let us also consider the map $\mathscr{F}_2$ of $L^2(\mathbb{R}^d_r \times \mathbb{R}^d_\xi, \mathbb{C})$ into $L^2(\mathbb{R}^d_r \times \mathbb{R}^d_p, \mathbb{C})$ given by

$$
(5.4) \qquad (\mathscr{F}_2 g)(r, p) := (2\pi)^{-d} \int_{\mathbb{R}^d_\xi} g(r, \xi)\, \mathrm{e}^{-ip\cdot\xi}\, d\xi \,,
$$

for all $g \in L^2(\mathbb{R}^d_r \times \mathbb{R}^d_\xi, \mathbb{C})$. Note that $\mathscr{F}_2$ is the Fourier transform with respect to the second group of variables, with the normalization constant $(2\pi)^{-d}$ instead of the standard $(2\pi)^{-d/2}$. Thus, Plancherel's theorem yields

$$
(5.5) \qquad \langle \mathscr{F}_2 g_1, \mathscr{F}_2 g_2 \rangle = (2\pi)^{-d} \langle g_1, g_2 \rangle
$$

for all g_1, g_2.

DEFINITION 5.1. – *The* Wigner transform *is the map*

$$
(5.6) \qquad \mathscr{W} := \mathscr{F}_2 \mathscr{R} : L^2(\mathbb{R}^d_x \times \mathbb{R}^d_y, \mathbb{C}) \to L^2(\mathbb{R}^d_r \times \mathbb{R}^d_p, \mathbb{C}).
$$

Explicitly:

$$
(5.7) \qquad (\mathscr{W}\varrho)(r, p) = (2\pi)^{-d} \int_{\mathbb{R}^d} \varrho\left(r + \frac{\hbar}{2}\xi, r - \frac{\hbar}{2}\xi\right) \mathrm{e}^{-ip\cdot\xi}\, d\xi
$$

for all $\varrho \in L^2(\mathbb{R}^d_x \times \mathbb{R}^d_y, \mathbb{C})$.

From eqs. (5.3) and (5.5) we obtain that

$$
(5.8) \qquad \langle \mathscr{W}\varrho_1, \mathscr{W}\varrho_2 \rangle = (2\pi\hbar)^{-d} \langle \varrho_1, \varrho_2 \rangle
$$

for all $\varrho_1, \varrho_2 \in L^2(\mathbb{R}^d_x \times \mathbb{R}^d_y, \mathbb{C})$, i.e., the Wigner transform is a unitary trasformation of $L^2(\mathbb{R}^{2d}, \mathbb{C})$ in itself, apart from the constant factor $(2\pi\hbar)^{-d}$. By using $(\mathscr{F}_2^{-1} w)(r, \xi) = \int_{\mathbb{R}^d} w(r, p)\, \mathrm{e}^{i\xi\cdot p}\, dp$ and (5.2), it is immediate to see that the

inverse Wigner transform $\mathbb{W}^{-1} = \mathcal{R}^{-1}\mathcal{F}_2^{-1}$ *is given by*

$$(5.9) \qquad (\mathbb{W}^{-1}w)(x,\, y) = \int_{\mathbb{R}^d} w\left(\frac{x+y}{2},\, p\right) e^{i(x-y)\cdot p/\hbar}\, dp$$

for all $w \in L^2(\mathbb{R}_r^d \times \mathbb{R}_p^d,\, \mathbb{C})$.

So far we have considered the Wigner transform of a generic function $\varrho \in L^2(\mathbb{R}_x^d \times \mathbb{R}_y^d,\, \mathbb{C})$. However, the ϱ's that interest us the most are those which represent quantum mechanical mixed states, i.e., density matrices/operators.

DEFINITION 5.2. – *A «physical Wigner function» (or, simply, «Wigner function») is the Wigner transform of a density matrix* [7].

For example, the Wigner transform of a pure state P_ψ is a Wigner function that will be denoted by w^ψ:

$$(5.10) \qquad\qquad w^\psi := \mathbb{W}P_\psi, \qquad \psi \in \mathcal{H}.$$

This is the most important example since from Theorem 4.2 it follows, by linearity, that every Wigner function is a convex combination of pure-state Wigner functions.

The following proposition gives another characterization of physical Wigner functions.

PROPOSITION 5.1. – *A function $w \in L^2(\mathbb{R}_r^d \times \mathbb{R}_p^d,\, \mathbb{C})$ is the Wigner transform of a density matrix ϱ if and only if it has the following properties:*

(P1) w is real;

(P2) $\displaystyle\int_{\mathbb{R}_r^d \times \mathbb{R}_p^d} w(r,\, p)\, dr\, dp = 1;$

(P3) $\displaystyle\int_{\mathbb{R}_r^d \times \mathbb{R}_p^d} w(r,\, p)\, w^\psi(r,\, p)\, dr\, dp \geq 0$, for all $\psi \in \mathcal{H}$.

PROOF. – Recalling Definition 4.1 and Theorems 4.1, 4.2 of Sec. 3, it is not difficult to prove that ϱ is a density matrix if and only if

(P1') $\varrho(x,\, y) = \overline{\varrho(y,\, x)}$, for all $x,\, y \in \mathbb{R}^d$;

(P2') $\displaystyle\int_{\mathbb{R}^d} \varrho(x,\, x)\, dx = 1;$

(P3') $\displaystyle\int_{\mathbb{R}_x^d \times \mathbb{R}_y^d} \varrho(x,\, y)\, \overline{\psi}(x)\, \psi(y)\, dx\, dy \geq 0$, for all $\psi \in \mathcal{H}$.

[7] Note that, if the density matrix $\varrho(x,\, y)$ has, as usual, the physical dimensions of a density in position space, then, the Wigner transform of ϱ has the physical dimensions of a density in phase-space.

Now, if $w = \mathcal{W}\varrho$, $\varrho = \mathcal{W}^{-1}w$, by using (5.1) and (5.9) we immediately see that (P1′) is equivalent to (P1). Moreover, if we compute $\int_{\mathbb{R}^d_r \times \mathbb{R}^d_p} w(r, p)\, dr\, dp$ and use the identity $(2\pi)^{-d} \int_{\mathbb{R}^d_p} e^{-ip\cdot\xi}\, dp = \delta(\xi)$, we can see that (P2′) is equivalent to (P2). Finally, by using (5.8) and denoting by ϱ^ψ the density matrix of the pure state P_ψ, we can write

$$\int_{\mathbb{R}^d_x \times \mathbb{R}^d_y} \varrho(x, y)\, \overline{\psi}(x)\, \psi(y)\, dx\, dy = \langle \varrho, \varrho^\psi \rangle_{L^2(\mathbb{R}^d_x \times \mathbb{R}^d_y, \mathbb{C})} = (2\pi\hbar)^d \langle w, w^\psi \rangle_{L^2(\mathbb{R}^d_r \times \mathbb{R}^d_p, \mathbb{C})} = $$

$$(2\pi\hbar)^d \int_{\mathbb{R}^d_r \times \mathbb{R}^d_p} w(r, p)\, w^\psi(r, p)\, dr\, dp$$

(where we also used the fact that w^ψ is real) and, therefore, (P3′) is equivalent to (P3). ∎

Analogously to wave functions (and density matrices), a Wigner function does not possess a direct physical meaning and physical information has to be extracted by taking expected values (see Axioms 2.3 and 4.2). To this aim, by using (3.7), (4.7) and (5.7), it is not difficult to prove the following important result.

PROPOSITION 5.2. – Let $\varrho \in L^2(\mathbb{R}^d_x \times \mathbb{R}^d_y, \mathbb{C})$ be a density matrix and let $w = \mathcal{W}\varrho \in L^2(\mathbb{R}^d_r \times \mathbb{R}^d_p, \mathbb{C})$ be the corresponding Wigner function. Moreover, let A_γ be the Weyl quantization of a symbol γ, such that ϱA_γ has finite trace. Then,

$$(5.11) \qquad \mathrm{Tr}(\varrho A_\gamma) = \int_{\mathbb{R}^d_r \times R^d_p} \gamma(r, p)\, w(r, p)\, dr\, dp\,.$$

From the discussion developed in the previous sections and, in particular, from eq. (4.9), we have that the above formula expresses expected values of measurements of observables in the Wigner picture. Here, the analogy with classical statistical mechanics is apparent; in fact, if w was a classical distribution in phase-space, eq. (5.11) would be the classical expectation of γ. However, w itself cannot be interpreted as a density. In fact, w is real, according to (P1), but *it is not necessarily non-negative*.

Nevertheless, the «marginal distributions of w» are true distributions. In fact, let $\mathcal{B} \subset \mathbb{R}^d_r$ and $\gamma(r, p) := \mathfrak{I}_{\mathcal{B}}(r)$. Thus, recalling the definition (3.1) of the position operator A_r and using (3.6), (4.8), (5.11) we get

$$\mathrm{Prob}\,[X_{A_r, \varrho} \in \mathcal{B}] = \mathrm{Tr}\,(\varrho\, \mathfrak{I}_{\mathcal{B}}(A_r)) = \mathrm{Tr}(\varrho A_\gamma) = \int_{\mathcal{B} \times \mathbb{R}^d_p} w(r, p)\, dr\, dp$$

which means that $r \mapsto \int_{\mathbb{R}_p^d} w(r, p) \, dp$ is the position density. This can also be verified directly by computing

$$(5.12) \qquad \int_{\mathbb{R}_p^d} w(r, p) \, dp = \varrho(r, r) = \sum_{j=1}^{\infty} \alpha_j \, |\phi_j(r)|^2$$

from (4.7). Analogously, we can verify that $p \mapsto \int_{\mathbb{R}_r^d} w(r, p) \, dr$ is the momentum density

$$(5.13) \qquad \int_{\mathbb{R}_r^d} w(r, p) \, dr = \widehat{\varrho}(p, p) = \sum_{j=1}^{\infty} \alpha_j \, |(\mathcal{F}\phi_j)(p)|^2.$$

In the last equation, $\widehat{\varrho}$ is the «density matrix in momentum representation»

$$(5.14) \qquad \widehat{\varrho}(p, q) := \sum_{j=1}^{\infty} \alpha_j (\mathcal{F}\phi_j)(p) \overline{(\mathcal{F}\phi_j)}(q)$$

(see (3.3) and (4.7)). The precise meaning of the integrals and diagonal traces appearing in eqs. (5.12) and (5.13) is discussed in Ref. [18], section II. We do not enter here in details.

REMARK 5.1. – In Sec. 3 we have remarked that P_ψ is an observable that has no classical counterpart (see Remark 3.1) and the same is true, more in general, for a density operator ϱ. Let $w = \mathcal{W}\varrho$ be the Wigner transform of ϱ. Then, by using (3.7), (4.4) and (5.9) we get the following interesting relation

$$(5.15) \qquad \varrho = A_{(2\pi\hbar)^d w}$$

which means that *the density operator is the Weyl quantization of the associated Wigner function* (times a constant factor $(2\pi\hbar)^d$). Thus, ϱ is not the quantization of any classical symbol because it is the quantization of the non-classical symbol w. Note also from eq. (5.15) that in some sense the Wigner transform and the Weyl quantization are inverse each other.   ∎

6. – The Wigner equation.

In the previous section we have introduced the Wigner formulation of QM. In particular, we have seen how mixed states and expected values of observables look like in such a formulation, which shows striking analogies with classical statistical mechanics.

We now turn our attention to the dynamical aspects. The aim of the present section is to deduce an evolution equation for the Wigner functions starting

from the evolution equation for density operators, i.e., from the Liouville equation (4.11).

In view of this, we focus now our attention on operators acting on a HS-operator (or, equivalently, on a HS-matrix) ϱ in the commutator form $[A, \varrho]$, where A is a linear operator on $\mathcal{H}$. The operator A is assumed to satisfy the following assumptions:

(A1) A is a linear operator on $\mathcal{H}$ with domain $\mathcal{D}(A)$;

(A2) $\mathcal{D}(A)$ is dense in $\mathcal{H}$;

(A3) A is closable.

Let us suppose for a moment that ϱ is a *density* operator; then, in this case, (4.7) holds and we can easily deduce

$$(6.1) \qquad [A, \varrho] = \sum_{j=1}^{\infty} \alpha_j \{ (A\phi_j) \otimes \phi_j - \phi_j \otimes (A^*\phi_j) \}.$$

Explicitly, the action on the density matrix is

$$(6.2) \qquad [A, \varrho](x, y) = \sum_{j=1}^{\infty} \alpha_j \left\{ (A\phi_j)(x)\, \overline{\phi_j(y)} - \phi_j(x) \overline{(A^*\phi_j)(y)} \right\}.$$

This suggests to re-define

$$(6.3) \qquad [A, \cdot] := A \otimes I - I \otimes A^*.$$

We recall (see Ref. [24], sec. VIII.10) that $A \otimes I - I \otimes A^*$ is defined as follows. For elements of the form $\psi \otimes \phi$, with $\psi \in \mathcal{D}(A)$ and $\phi \in \mathcal{D}(A^*)$, we put

$$(6.4) \qquad (A \odot I - I \odot A^*)(\psi \otimes \phi) := (A\psi) \otimes \phi - \psi \otimes (A^*\phi).$$

Then, the definition is linearly extended to the subspace $\mathcal{D}(A) \odot \mathcal{D}(A^*)$ of finite linear combinations of such elements. Under the assumptions (A1)-(A3), such subspace is dense in $\mathcal{H} \otimes \mathcal{H}$ and the operator $A \odot I - I \odot A^*$ with domain $\mathcal{D}(A) \odot \mathcal{D}(A^*)$ is closable. Thus, the operator $A \otimes I - I \otimes A^*$ is defined as the closure of $A \odot I - I \odot A^*$.

We can now prescribe a «canonical way» of associating to an operator A acting on $\mathcal{H}$ (i.e., on the pure-state space) an operator A^{wig} acting on Wigner functions (or, more in general, to functions belonging to $L^2(\mathbb{R}_r^d \times \mathbb{R}_p^d, \mathbb{C})$). We recall that $\mathcal{W}$ denotes the Wigner transform (see Definition 5.1).

DEFINITION 6.1. – *For every A satisfying the assumptions* (A1)-(A3) *we define the operator*

(6.5) $A^{\mathrm{wig}} := \mathcal{W}[A, \cdot]\, \mathcal{W}^{-1} \colon \mathcal{D}(A^{\mathrm{wig}}) \subseteq L^2(\mathbb{R}_r^d \times \mathbb{R}_p^d, \mathbb{C}) \to L^2(\mathbb{R}_r^d \times \mathbb{R}_p^d, \mathbb{C}),$

where $[A, \cdot] := A \otimes I - I \otimes A^*$ *and* $\mathcal{D}(A^{\mathrm{wig}}) := \mathcal{W}\mathcal{D}([A, \cdot])$.

We shall call A^{wig} the «wignerization» of A. Let us illustrate the wignerization of two significant categories of operators: the constant coefficient differential operators and the multiplication operators. In the examples we shall proceed in a formal way, disregarding questions concerning the domains.

EXAMPLE 6.1 (Constant coefficient differential operators). – We look for the wignerization of a constant coefficient differential operator D of the form

$$(6.6) \qquad\qquad D := \sum_{|k| \leqslant n} c_k \partial_x^k,$$

where the coefficients c_k are complex constants and $n \in \mathbb{N} \cup \{0\}$ is the degree of D. Here we are using the multi-index convention: if $k = (k_1, \ldots, k_d)$ is a d-uple of non-negative integers, we put

$$(6.7) \qquad\qquad \partial_x^k := \frac{\partial^{k_1}}{\partial x_1^{k_1}} \frac{\partial^{k_2}}{\partial x_2^{k_2}} \cdots \frac{\partial^{k_d}}{\partial x_d^{k_d}}$$

and $|k| := k_1 + k_2 + \ldots + k_d$. By using (6.1) we obtain the expression for $[D, \cdot]$:

$$(6.8) \qquad\qquad [D, \cdot] = \sum_{|k| \leqslant n} c_k (\partial_x^k - (-1)^{|k|} \partial_y^k).$$

Now, from (5.1) it follows that

$$\mathcal{R} \, \partial_x \mathcal{R}^{-1} = \frac{\partial_r}{2} + \frac{\partial_\xi}{\hbar} \quad \text{and} \quad \mathcal{R} \, \partial_y \mathcal{R}^{-1} = \frac{\partial_r}{2} - \frac{\partial_\xi}{\hbar}$$

and from (5.4)

$$\mathcal{W} \, \partial_x \mathcal{W}^{-1} = \frac{\partial_r}{2} + \frac{ip}{\hbar} \quad \text{and} \quad \mathcal{W} \, \partial_y \mathcal{W}^{-1} = \frac{\partial_r}{2} - \frac{ip}{\hbar} \, ,$$

where p denotes the vector of multiplication oparators, by $p_1, p_2, \ldots, p_d$. By exploiting linearity and the commutativity of ∂_r and p, from (6.8) we finally obtain the wignerization D^{wig} of D:

$$(6.9) \qquad D^{\text{wig}} = \sum_{|k| \leqslant n} c_k \left\{ \left(\frac{\partial_r}{2} + \frac{ip}{\hbar} \right)^k - (-1)^{|k|} \left(\frac{\partial_r}{2} - \frac{ip}{\hbar} \right)^k \right\}. \qquad \blacksquare$$

As a particular case of the above example, let us consider the quantum-mechanical kinetic energy operator

$$(6.10) \qquad\qquad A_{p^2/2m} = - \frac{\hbar^2}{2m} \Delta \, ,$$

where $\varDelta$ is the Laplace operator which is of the form (6.6) with

(6.11)
$$c_k = \begin{cases} 1 , & \text{if } k = (2, 2, ..., 2), \\ 0 , & \text{otherwise}. \end{cases}$$

Thus, from eq. (6.9) we obtain that *in the Wigner representation the kinetic energy operator is a free-streaming operator*, namely

(6.12)
$$A_{p^2/2m}^{\text{wig}} = -\frac{i\hbar}{m} p \cdot \partial_r.$$

EXAMPLE 6.2 (Multiplication operators). – Consider a (complex) function $V = V(x)$ and let A_V indicate the corresponding multiplication operator on $\mathcal{H}$:

(6.13)
$$(A_V \psi)(x) := V(x) \psi(x), \qquad x \in \mathbb{R}_x^d$$

(let us observe that the notation A_V is consistent with the definition (3.7)). By (6.1) we have that $[A_V, \cdot]$, acting on $L^2(\mathbb{R}_x^d \times \mathbb{R}_y^d, \mathbb{C})$, is the multiplication operator by $V(x) - V(y)$. Then, from (5.1) we easily obtain that $\mathcal{R}[A_V, \cdot] \mathcal{R}^{-1}$, acting on $L^2(\mathbb{R}_r^d \times \mathbb{R}_\xi^d, \mathbb{C})$, is the multiplication by the function

(6.14)
$$\delta V(r, \xi) := V\left(r + \frac{\hbar}{2}\xi\right) - V\left(r - \frac{\hbar}{2}\xi\right).$$

After the application of the subsequent transformation $\mathcal{F}_2$, see (5.4), we finally obtain that the wignerization of the multiplication operator A_V is given by the pseudo-differential operator, [13],

(6.15)
$$A_V^{\text{wig}} = \delta V(r, -i\partial_p),$$

i.e., explicitly,

(6.16) $$(A_V^{\text{wig}} w)(r, p) = (2\pi)^{-d} \int_{\mathbb{R}_\xi^d \times \mathbb{R}_{p'}^d} \delta V(r, \xi) w(r, p') e^{-i(p - p') \cdot \xi} d\xi \, dp'.$$

Note that the right hand side of (6.16) can be put in the convolution form

(6.17) $$(A_V^{\text{wig}} w)(r, p) = \int_{\mathbb{R}_{p'}^d} (\mathcal{F}_2 \delta V)(r, p - p') w(r, p') \, dp'.$$

After a little algebra, and assuming V real, we can relate the convolution ker-

nel with the Fourier transform of the function V:

$$(6.18) \quad (\mathcal{F}_2 \delta V)(r, p) := \begin{cases} \left(\dfrac{2}{\pi\hbar}\right)^{d/2} 2\,\mathrm{Re}\,[e^{2ip\cdot r/\hbar}(\mathcal{F}V)(2p)] & \text{if } d \text{ is odd,} \\[2ex] \left(\dfrac{2}{\pi\hbar}\right)^{d/2} 2\,\mathrm{Im}\,[e^{2ip\cdot r/\hbar}(\mathcal{F}V)(2p)] & \text{if } d \text{ is even.} \end{cases} \qquad \blacksquare$$

It is now possible to write the dynamical equations for the Wigner functions. From the previous discussion it follows that, if the density operator ϱ satisfies the quantum Liouville equation (4.11), then, the corresponding Wigner function $w := \mathcal{W}\varrho$ satisfies the evolution equation

$$(6.19) \qquad\qquad i\hbar\frac{d}{dt}w(t) = H^{\mathrm{wig}}w(t), \quad t \in \mathbb{R}$$

in the Hilbert Space $L^2(\mathbb{R}^d_r \times \mathbb{R}^d_p, \mathbb{C})$, where H^{wig} is the wignerization of the Hamiltonian H on $\mathcal{H}$, according to Definition 6.1. Let us consider a typical Hamiltonian of the form

$$(6.20) \qquad\qquad H = A_{p^2/2m} + A_V,$$

where $A_{p^2/2m}$ is the kinetic energy operator (6.10) and A_V is the potential energy operator (V is the potential energy function). From eqs. (6.12) and (6.15) it follows that

$$(6.21) \qquad H^{\mathrm{wig}} = A^{\mathrm{wig}}_{p^2/2m} + A^{\mathrm{wig}}_V = -\frac{i\hbar}{m}p\cdot\partial_r + \delta V(r, -i\partial_p).$$

Therefore, the evolution equation (6.19) takes the specific form

$$(6.22) \qquad \frac{\partial}{\partial t}w(t) + \frac{p}{m}\cdot\partial_r w(t) + \frac{i}{\hbar}\delta V(r, -i\partial_p)\,w(t) = 0,$$

which is known as *Wigner equation* [8].

Eq. (6.22) confirms, at the level of dynamical equations, the analogy between the Wigner formulation of QM and the classical statistical mechanics. In fact, we recall that a classical statistical ensemble $f(r, p, t)$, subject to a potential V, evolves in time according to the Liouville equation, [17],

$$(6.23) \qquad \frac{\partial}{\partial t}f(t) + \frac{p}{m}\cdot\partial_r f(t) - \partial_r V\cdot\partial_p\,f(t) = 0.$$

Note that the main formal difference between eq. (6.22) and eq. (6.23) is in the

[8] See Refs. [18, 20] for a discussion of the well-posedness of the initial-value problem for eq. (6.22).

potential term, which in the former is given by the pseudo-differential opera-
tor (6.16).

One of the main results on the Wigner equation (6.22) is that it reduces to
Louville equation (6.23), i.e., it gives classical dynamics, in the classical limit
$\hbar \to 0$. The reader can readily check this by noting that, formally,

$$\frac{i}{\hbar(2\pi)^d} \int_{\mathbb{R}_\xi^d \times \mathbb{R}_{p'}^d} \delta V(r, \xi)\, w(r, p')\, e^{-i(p - p') \cdot \xi}\, d\xi\, dp' \to -\partial_r V \cdot \partial_p\, w(r, p)$$

as $\hbar \to 0$. For a precise mathematical statement and proof of this result the
reader is referred to the paper of Lions and Paul, [18].

In conclusion we leave the reader with an exercise: prove that for quadrat-
ic potentials, i.e., potentials of the form

$$V(r) = \frac{1}{2} \sum_{i, j = 1}^d a_{ij}\, r_i\, r_j + \sum_{i = 1}^d b_i\, r_i + c$$

with $a_{ij}, b_i, c \in \mathbb{R}$ for $i, j = 1, \ldots d$, the pseudo-differential operator $\delta V(r, -i\partial_p)$
reduces to the operator $i\hbar\partial_r V \cdot \partial_p$ and, therefore, the Wigner equation is for-
mally identical to the classical Liouville equation.

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